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ME469: Variable Density/Property

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U.S. DEPARTMENT OF ENERGY

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What is a Variable-Density/Variable-Property Flow?

- Property changes due to energy and species transport, e.g., density, viscosity, mass diffusivity, etc.
- Common examples?
  - Hot/cold jets, fire, plumes, reacting flows (methane and coal combustion), liquids (multi-phase, for another class), etc.
- How are equations affected?

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j}\right) - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right] = -\frac{\partial p^m}{\partial x_i} + F_i$$

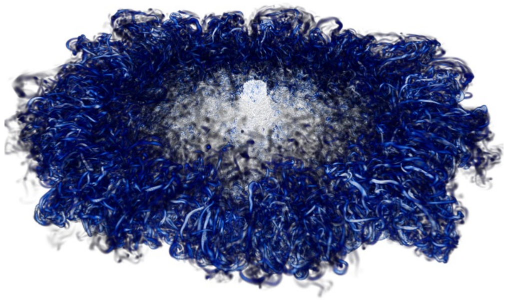
$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\frac{\mu}{Sc}\frac{\partial \phi}{\partial x_j} = S_\phi$$

$$\rho = f(\phi)$$

$$\mu = f(\phi)$$

Example: Heated Jet

- Property changes due to energy transport, e.g., density and viscosity
- How are equations affected?



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$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\mu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \right] = -\frac{\partial p^m}{\partial x_i} + F_i$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} - \frac{\partial}{\partial x_j}\frac{\mu}{Pr}\frac{\partial h}{\partial x_j} = 0$$

Unity Lewis number approximation

$$\rho = \frac{P^t M}{RT}$$

Ideal gas law

$$\mu(T) = \mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\frac{3}{2}} \frac{T_{ref} + S}{T + S}$$

Sutherlands law

Example: Heated Jet, Dive on Unity Lewis Number

- Common Assumption: Unity Lewis number, i.e., energy and species diffuse equally (not true for many systems, e.g., Hydrogen gas) where species mass diffusional flux need not be proportional to a species mass fraction gradient

$$Le = \frac{Sc}{Pr} = \frac{\alpha}{D} \qquad \alpha = \frac{\kappa}{\rho c_p} \qquad \mathrm{Pr} = \frac{c_p \mu}{\kappa} = \frac{\mu}{\rho \alpha} \qquad \mathrm{Sc} = \frac{\mu}{\rho D}$$

Useful relationship

$$\boxed{\begin{aligned} \frac{\partial h}{\partial x_j} &= \sum_{k=1}^{K} Y_k {C_p}_k \frac{\partial T}{\partial x_j} + \sum_{k=1}^{K} h_k \frac{\partial Y_k}{\partial x_j} \\ &= C_p \frac{\partial T}{\partial x_j} + \sum_{k=1}^{K} h_k \frac{\partial Y_k}{\partial x_j}. \end{aligned}}$$

- Energy diffusion vector (simplified) is written as:

$$q_j = -\kappa \frac{\partial T}{\partial x_j} + \sum_{k=1}^{K} h_k j_{j,k}$$

(second term: energy due to mass diffusion)

- Where species mass diffusional flux $j_{j,k} = \rho Y_k \hat{u}_{j,k}$ is related to the mass fraction and species mass diffusion velocity: $\hat{u}_{j,k} \equiv u_{j,k} - u_j$

Yielding:

$$q_j = -\frac{\kappa}{C_p} \left(\frac{\partial h}{\partial x_j} - \sum_{k=1}^{K} h_k \frac{\partial Y_k}{\partial x_j} \right) + \sum_{k=1}^{K} \rho h_k Y_k \hat{u}_{j,k}$$

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Useful relationship

$$\boxed{\begin{aligned}\frac{\partial h}{\partial x_j} &= \sum_{k=1}^{K} Y_k C_{p\,k} \frac{\partial T}{\partial x_j} + \sum_{k=1}^{K} h_k \frac{\partial Y_k}{\partial x_j} \\ &= C_p \frac{\partial T}{\partial x_j} + \sum_{k=1}^{K} h_k \frac{\partial Y_k}{\partial x_j}.\end{aligned}}$$

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For a Fickian mass diffusion velocity:

$$\hat{u}_{j,k} = -D \frac{1}{Y_k} \frac{\partial Y_k}{\partial x_j}$$

When Le = 1, terms cancel

Example: Helium Plume

- Property changes due to species transport, e.g., density and viscosity
- How are equations affected?
- Here, shown to be written in terms of a conserved mixture fraction variable, Z, rather than a set of species mass fractions, Y_k

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j}\right) - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right] = -\frac{\partial p^m}{\partial x_i} + F_i$$

$$\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} - \frac{\partial}{\partial x_j}\frac{\mu}{Sc}\frac{\partial Z}{\partial x_j} = 0 \qquad \rho = \frac{1}{\frac{Z}{\rho^p} + \frac{(1-Z)}{\rho^s}}$$

$$\mu(Z) = Z\mu^p + (1-Z)\mu^s$$

"p" primary
"s" secondary

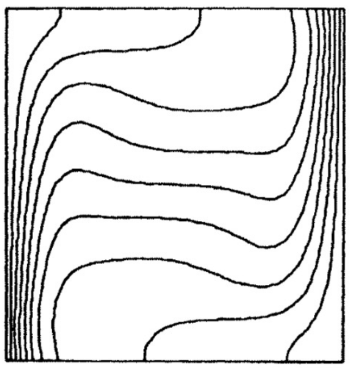
Intermediate Assumption: Boussinesq Approximation

- Density is constant; viscosity may vary
  - Equation shown below neglects temperature effects
  - Momentum stress tensor will lack the “div-u” contribution
- Source term, ρg_i approximated via $\rho = \rho_o - \beta(T - T_o)$ with, for an ideal gas, $\beta = 1/T_o$

$$\frac{\partial u_j}{\partial x_j} = 0,$$

$$\rho^o \frac{\partial u_i}{\partial x_j} + \rho^o \frac{\partial u_j u_i}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} = -\frac{\partial p^m}{\partial x_i} - \rho^o \beta \left(T - T^o\right) g_i,$$

$$\rho^o \frac{\partial h}{\partial t} + \rho^o \frac{\partial u_j h}{\partial x_j} - \frac{\mu}{Pr} \frac{\partial^2 h}{\partial x_j^2} = 0$$



De Vahl Davis, “NATURAL CONVECTION OF AIR IN A SQUARE CAVITY A BENCH MARK NUMERICAL SOLUTION”, Int. J. Numer. Method. Fluids (1983)

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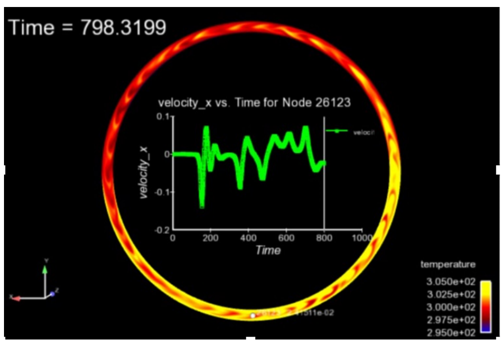

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$$\rho^o \frac{\partial h}{\partial t} + \rho^o \frac{\partial u_j h}{\partial x_j} - \frac{\mu}{Pr} \frac{\partial^2 h}{\partial x_j^2} = 0$$

- As with the “hula-hoop” example, water can be used
- Good approximation for buoyancy

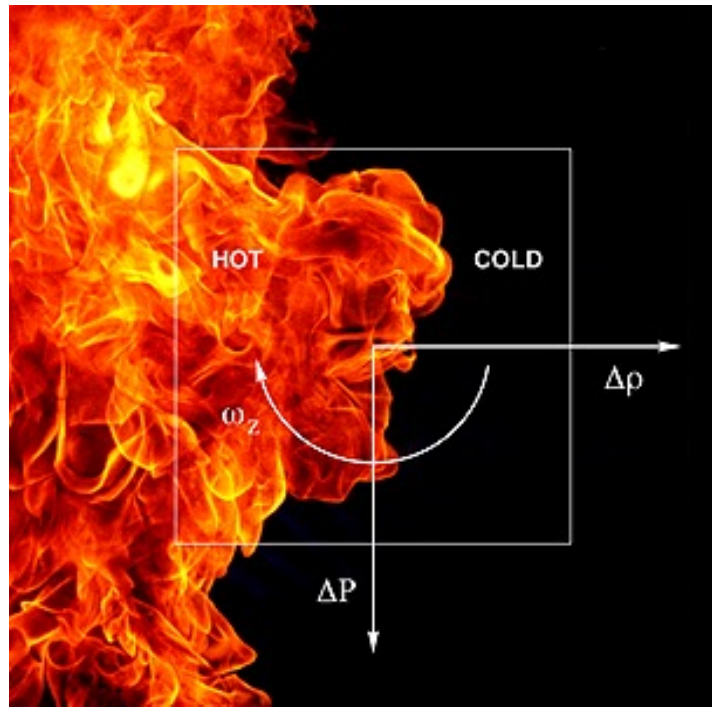
When Does the Boussinesq Approximation Fail? And Why?

- Fails for $\frac{\Delta\rho}{\rho} \sim 1$
- Valid for low Atwood numbers, $A_t = {\rho_a - \rho_b}/{\rho_a + \rho_b}$ (for helium/air, A_t ~ 0.75)

Baroclinic Torque: misaligned density and pressure gradients:

$$\frac{\nabla\rho \times \nabla p}{\rho^2}$$

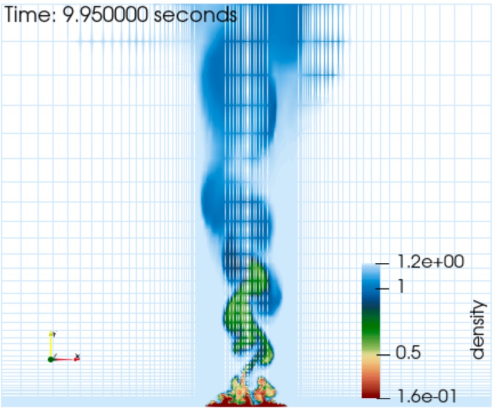
- This term is found by taking the cross product of the momentum equation to derive the vorticity transport equation



When Does the Boussinesq Approximation Fail?

- Therefore, the working equations for our helium plume laboratory at near unity Atwood numbers are as follows:

2D Laboratory



3D DNS

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

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$$\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} - \frac{\partial}{\partial x_j}\frac{\mu}{Sc}\frac{\partial Z}{\partial x_j} = 0$$

$$\rho = \frac{1}{\frac{Z}{\rho^p} + \frac{(1-Z)}{\rho^s}}$$

$$\mu(Z) = Z\mu^p + (1-Z)\mu^s$$

"p" primary
"s" secondary

2D slice of 1 meter helium plume

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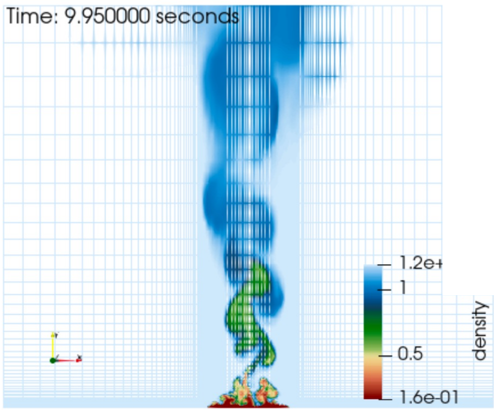

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$$\rho = \frac{1}{\frac{Z}{\rho^p} + \frac{(1-Z)}{\rho^s}}$$

$$\mu(Z) = Z\mu^p + (1-Z)\mu^s$$

"p" primary
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Note: Buoyancy term can subtract the hydrostatic contribution:

$$F_i = (\rho - \rho^{ref})g_i$$

2D slice of 1 meter helium plume

Ramifications: More Equations to Solve/Couple

- Implicit Monolithic (lower left) vs Segregated (lower right)
- Explicit, multi-stage RK schemes also are widely used

For a given time step:

do while (!converged) {

$$\begin{bmatrix} \frac{\partial}{\partial p}C & \frac{\partial}{\partial \tilde{u}_x}C & \frac{\partial}{\partial \tilde{u}_y}C & \frac{\partial}{\partial \tilde{z}}C \\ \frac{\partial}{\partial p}\tilde{U}_x & \frac{\partial}{\partial \tilde{u}_x}\tilde{U}_x & \frac{\partial}{\partial \tilde{u}_y}\tilde{U}_x & \frac{\partial}{\partial \tilde{z}}\tilde{U}_x \\ \frac{\partial}{\partial p}\tilde{U}_y & \frac{\partial}{\partial \tilde{u}_x}\tilde{U}_y & \frac{\partial}{\partial \tilde{u}_y}\tilde{U}_y & \frac{\partial}{\partial \tilde{z}}\tilde{U}_y \\ \frac{\partial}{\partial p}\tilde{Z} & \frac{\partial}{\partial \tilde{u}_x}\tilde{Z} & \frac{\partial}{\partial \tilde{u}_y}\tilde{Z} & \frac{\partial}{\partial \tilde{z}}\tilde{Z} \end{bmatrix} \begin{bmatrix} \Delta p \\ \Delta \tilde{u}_x \\ \Delta \tilde{u}_y \\ \Delta \tilde{z} \end{bmatrix} = - \begin{bmatrix} resC \\ res\tilde{U}_x \\ res\tilde{U}_y \\ res\tilde{Z} \end{bmatrix}$$

}

do while (!converged) {

$$\begin{bmatrix} \frac{\partial}{\partial p}C & \cancel{\frac{\partial}{\partial \tilde{u}_x}C} & \cancel{\frac{\partial}{\partial \tilde{u}_y}C} & \cancel{\frac{\partial}{\partial \tilde{z}}C} \\ \cancel{\frac{\partial}{\partial p}\tilde{U}_x} & \frac{\partial}{\partial \tilde{u}_x}\tilde{U}_x & \cancel{\frac{\partial}{\partial \tilde{u}_y}\tilde{U}_x} & \cancel{\frac{\partial}{\partial \tilde{z}}\tilde{U}_x} \\ \cancel{\frac{\partial}{\partial p}\tilde{U}_y} & \cancel{\frac{\partial}{\partial \tilde{u}_x}\tilde{U}_y} & \frac{\partial}{\partial \tilde{u}_y}\tilde{U}_y & \cancel{\frac{\partial}{\partial \tilde{z}}\tilde{U}_y} \\ \cancel{\frac{\partial}{\partial p}\tilde{Z}} & \cancel{\frac{\partial}{\partial \tilde{u}_x}\tilde{Z}} & \cancel{\frac{\partial}{\partial \tilde{u}_y}\tilde{Z}} & \frac{\partial}{\partial \tilde{z}}\tilde{Z} \end{bmatrix} \begin{bmatrix} \Delta p \\ \Delta \tilde{u}_x \\ \Delta \tilde{u}_y \\ \Delta \tilde{z} \end{bmatrix} = - \begin{bmatrix} resC \\ res\tilde{U}_x \\ res\tilde{U}_y \\ res\tilde{Z} \end{bmatrix}$$

}

Monolithic, or fully-coupled: One System, One Matrix inversion (Left)
Segregated: Multiple Systems

Pressure Projection For Variable Density

- Semi-discrete approach (uniform density)

$$\rho\frac{\hat{u}_i-u_i^n}{\Delta t}+\frac{\partial}{\partial x_j}\left(\rho\hat{u}_i u_j^n\right)=-\frac{\partial p^n}{\partial x_i}+\frac{\partial\hat{\tau}_{ij}}{\partial x_j}$$

$$\rho\frac{u_i^{n+1}-\hat{u}_i}{\Delta t}=-\frac{\partial}{\partial x_i}\left(p^{n+1}-p^n\right)$$

$$\frac{\partial^2}{\partial x_i^2}\left(p^{n+1}-p^n\right)=\frac{\rho}{\Delta t}\frac{\partial\hat{u}_i}{\partial x_i}$$

  - Chorin (1968)
  - Time scale is the time step:

$$u_i^{n+1}=\hat{u}_i-\Delta t\left(\frac{1}{\rho}\frac{\partial}{\partial x_i}\left(p^{n+1}-p^n\right)\right)$$

- Fully discrete approach

$$\begin{bmatrix}\mathbf{A} & \mathbf{G}\\ \mathbf{D} & \mathbf{0}\end{bmatrix}\begin{Bmatrix}\mathbf{U}^{n+1}\\ \mathbf{P}^{n+1}\end{Bmatrix}=\begin{Bmatrix}\mathbf{f}\\ \mathbf{0}\end{Bmatrix}$$

  - Factored matrix:

$$\begin{bmatrix}\mathbf{A} & \mathbf{G}\\ \mathbf{D} & \mathbf{0}\end{bmatrix}\approx\begin{bmatrix}\mathbf{A} & \mathbf{0}\\ \mathbf{D} & -\mathbf{D}\bar{\mathbf{A}}^{-1}\mathbf{G}\end{bmatrix}\begin{bmatrix}\mathbf{I} & \bar{\mathbf{A}}^{-1}\mathbf{G}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}$$

  $\bar{\mathbf{A}}^{-1}$ is an approximation to $\mathbf{A}^{-1}$

  - SIMPLE family of methods
  - Time scale is the characteristic scale of $\bar{\mathbf{A}}^{-1}$:

$$\mathbf{U}^{n+1}=\hat{\mathbf{U}}-\bar{\mathbf{A}}^{-1}\mathbf{G}\mathbf{P}^{n+1}$$

    - For convection-dominated flows, this looks like Δx/U

$$\begin{bmatrix}\boldsymbol{A} & \boldsymbol{G}\\ \boldsymbol{D} & 0\end{bmatrix}\begin{bmatrix}u^{n+1}\\ p^{n+1}\end{bmatrix}=\begin{bmatrix}\boldsymbol{f}\\ 0\end{bmatrix}+\begin{bmatrix}(\boldsymbol{I}-\boldsymbol{A}\tau)\boldsymbol{G}(p^{n+1}-p^n)\\ \tau(\boldsymbol{L}-\boldsymbol{D}\boldsymbol{G})(p^{n+1}-p^n)\end{bmatrix}$$

Pressure Projection For Variable Density

- Semi-discrete approach (variable density)

$$\frac{\rho^* \hat{u}_i - \rho^n u_i^n}{\Delta t} + \frac{\partial}{\partial x_j}\left(\rho^* u_j^* \hat{u}_i\right) = -\frac{\partial p^*}{\partial x_i} + \frac{\partial \hat{\tau}_{ij}}{\partial x_j},$$

$$-\frac{\partial^2}{\partial x_j^2}\left(p^{n+1} - p^*\right) = -\frac{1}{\Delta t}\left(\frac{\rho^* - \rho^n}{\Delta t} + \frac{\partial \rho^* u_j^*}{\partial x_j}\right),$$

$$u_i^{n+1} = u_i^* - \frac{\Delta t}{\rho^*}\left(\frac{p^{n+1} - p^*}{\partial x_i}\right)$$

- Fully discrete approach

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{U}^{n+1} \\ \mathbf{P}^{n+1} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f} \\ \mathbf{0} \end{Bmatrix}$$

  - Factored matrix:

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \approx \begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{D} & -\mathbf{D}\bar{\mathbf{A}}^{-1}\mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \bar{\mathbf{A}}^{-1}\mathbf{G} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}$$

  $\bar{\mathbf{A}}^{-1}$ is an approximation to $\mathbf{A}^{-1}$

  - SIMPLE family of methods
  - Time scale is the characteristic scale of $\bar{\mathbf{A}}^{-1}$:

$$\mathbf{U}^{n+1} = \hat{\mathbf{U}} - \bar{\mathbf{A}}^{-1}\mathbf{G}\mathbf{P}^{n+1}$$

    - For convection-dominated flows, this looks like $\Delta x/U$

D operator now Includes density scaling

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{G} \\ \boldsymbol{D} & 0 \end{bmatrix} \begin{bmatrix} u^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ 0 \end{bmatrix} + \begin{bmatrix} (\boldsymbol{I} - \boldsymbol{A}\tau)\boldsymbol{G}(p^{n+1} - p^n) \\ \tau(\boldsymbol{L} - \boldsymbol{D}\boldsymbol{G})(p^{n+1} - p^n) \end{bmatrix}$$

Special Ordering

Order can be changed to increase convergence and consistency

"predictor/corrector" approaches are common

Shunn et al., JCP, 2012

For a given time step:

do while (!converged) {

$$\bar{\rho} = f(\tilde{Z})$$

$$\left[\frac{\partial}{\partial \tilde{u}_x}\tilde{U}_x\right]\left[\Delta \tilde{u}_x\right] = -\left[res\tilde{U}_x\right]$$

$$\left[\frac{\partial}{\partial \tilde{u}_y}\tilde{U}_y\right]\left[\Delta \tilde{u}_y\right] = -\left[res\tilde{U}_y\right]$$

$$\tilde{u}_i^{k+1} = \tilde{u}_i^k + \alpha \Delta \tilde{u}_i$$

$$\left[\frac{\partial}{\partial p}C\right]\left[\Delta p\right] = -\left[resP\right]$$

$$\tilde{u}_i^{n+1} = \tilde{u}_i^{k+1} - \tau \nabla (\Delta p^{n+1/2})$$

$$\left[\frac{\partial}{\partial \tilde{z}}\tilde{Z}\right]\left[\Delta \tilde{z}\right] = -\left[res\tilde{Z}\right]$$

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$$\bar{\rho} = f(\tilde{Z})$$

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}

Other Ramifications: Properties to Interpolate to Integration Points

Advection and Diffusion Example

- Element-based (same applies for the two-state schemes)

$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$

$$\int w \frac{\partial q_j}{\partial x_j} dV \approx -\sum_{ip} \frac{\mu}{Sc}_{ip} \frac{\partial \phi}{\partial x_j}_{ip} n_j dS = -\sum_{ip} \frac{\mu}{Sc}_{ip} \sum_{nd} \frac{\partial N^{ip}_{nd}}{\partial x_j} \phi_{nd} A^{ip}_j$$

- Sometimes, a code implementation chooses to express properties, even when constant, as interpolated – solely for generality of implementation

Final Points

- Variable density flows with property variations will includes additional transport equations
  - Mixture fraction, species, energy transport, etc.
- The momentum system may also include new body force source terms
- An intermediate approach is the so-called Boussinesq approximation where a body force is added to momentum, while it is assumed that density variations can be neglected
  - Fails as density difference increases, $\frac{\Delta\rho}{\rho} \sim 1$
- Additional equations means new complexities in the nonlinear solver
- The hula hoop and helium plume cases are good samples to explore the effect of variable density flows